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## Mole Street Journal, September 2014

University of Arkansas, Fayetteville. Dept. of Chemistry and Biochemistry

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# The Mole Street Journal

Department of Chemistry and Biochemistry

Volume 13, Issue 9

September 2014

## Special points of interest:

- New faculty arrive
- Change in department leadership
- Ayinuola recruits at ACS meeting
- Graduate students attend Conclave

## Inside this issue:

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## Department Welcomes 16 New Graduate Students



The Department of Chemistry and Biochemistry is very pleased to introduce to you our 16 new graduate students. Starting with the back row in the picture above (l-r):

Qile Wang, China, BS Sun-Yat-Sen University  
Elvis Boateng, Ghana, BS University of Ghana, MS Texas A&M  
Perry Caviness, Arkansas, BS University of Arkansas  
Joel Baker, Missouri, BS Missouri Southern State University

Middle row (l-r):

Zhijian Hu (CeMB), China, BS and MS Tongui Medical College of Huazhong University of Science and Technology  
Zainab Almansaf, Saudi Arabia, BSc University of Dammam  
Mamello Mohale, Lesotho, BS and MS, Rhodes University  
Mahsa Lotfi-Marchoubbeh, Iran, BS and MS Isfahan University of Technology  
Anthony Emerson, Arkansas, BS Southern Arkansas University

Front row (l-r):

Djamali Muhoza (CeMB), Rwanda, BA Hendrix College  
Fahmida Afrose, Bangladesh, BS and MS University of Dhaka  
Julie Davis, Arkansas, BS University of Central Arkansas  
Erika Bass, Arkansas, BS Henderson State University  
Jessica Pickens, Arkansas, BS University of Arkansas at Fort Smith  
Matthew McKay, Maine, BS Ursinus College

Pictured above at right:

Anh Nguyen, Viet Nam, BS Vietnam National University, MS Purdue University



## Faculty News

### On the Go

**Feng Wang's** laboratory group presented three posters at the American Conference on Theoretical Chemistry, July 20-25, 2014 in Telluride, Colorado. "Pairwise-additive Force Field for Ions from Adaptive Force Matching," **Jicun Li** and **Feng Wang**. "A Polarizable Water Model Developed with the Adaptive Force Matching Method," **Saieswari Amaran, Tomasz Janowski, Peter Pulay, Revati Kumar, Tom Keyes,** and **Feng Wang**. "On the Transferability of Three Water Models Developed by Adaptive Force Matching (AFM)," **Hongyi Hu, Zhonghua Ma,** and **Feng**

### Wang.

Tomasz Janowski gave an oral presentation at the 248th ACS National Meeting in San Francisco: **T. Janowski** and **P. Pulay**, "Localized Laplace Transformed Coupled Cluster Laplace Transformed Perturbative Triples Correction in Quasiatomic Orbitals." At the same meeting, Peter Pulay gave an invited oral presentation: **P. Pulay, T. Janowski, K. Wolinski**, "Generalized Multipole Polarizabilities and their use in Ultrafast AM/MM Simulations."

### Recognition

**Paul Adams** received notification from the Arkansas Science & Tech-

nology Authority (ASTA) that his project "Characterization of the Novel Features of Interactions Involving the Ras-Related Protein, Rheb, and Tuberous Sclerosis Complex 2," was funded for a period of one year. He also was invited to speak on a diversity panel during the 4th Annual Arkansas ASSET Initiative Project Meeting to be held September 5, 2014. Arkansas ASSET Initiative is a National Science Foundation EPSCoR project composed of 3 research themes: Biotechnology, Solar Energy and Grid-Integration for Renewable Energy.

## New Faculty



**Stefan Kilyanek** spent his formative years in western Michigan. He earned his B.S. in Chemistry from Grand Valley State University in Allendale, MI. Kilyanek earned an M.S. in 2004 and Ph.D. in 2009 from the University of Chicago working with Prof. Richard F. Jordan. From 2010 to 2014, he was a postdoctoral researcher at the Massachusetts Institute of Technology with Prof. Richard R. Schrock and Prof. Yogesh Surendranath. In graduate school, Kilyanek studied the mechanisms of organometallic olefin polymerization catalysts using NMR spectroscopy and Density Functional Theory. As a postdoc with Prof. Schrock, Kilyanek worked extensively on the synthesis and study of reactive compounds including olefin metathesis catalysts and the mechanisms of stereo-regular polymerization. During his time with Prof. Surendranath, Kilyanek studied the interfacial chemistry of carbon electrodes and their modification with organic and organometallic compounds. Kilyanek's independent research program will revolve around solving problems in organometallic and inorganic catalysis using an interdisciplinary approach. His group will combine organic and inorganic synthesis, molecular modeling, materials science, and electrochemistry. His areas of interest include small molecule activation by multi-metallic complexes and electrochemically driven inorganic catalysis for the production of fuels from biomass-

derived sources. During his visits, he was impressed by the quality of the students in the department as well as the collegial and friendly environment.

**Margaret Hershberger** grew up in southwestern Ohio. She earned her B.S. degrees in Chemistry and Mathematics from the Ohio State University. As a graduate student with Prof. Norbert F. Scherer, Hershberger used nonlinear spectroscopy to study solvation dynamics and earned her M.S. and Ph.D. degrees from the University of Chicago. She then continued to study liquid dynamics with Prof. Richard M. Stratt at Brown University and joined the faculty at Brown as a visiting lecturer. Hershberger has an established interest in teaching chemistry. In particular, she has experience with general chemistry support programs and classes for students with a variety of backgrounds. At the University of Chicago, she developed a collaborative chemistry study program for undergraduate students from Chicago public and parochial schools. At Brown, Hershberger contributed to the ongoing development of collaborative problem solving sessions for students to build their math and chemistry skills. She is excited to join the department at the University of Arkansas as an instructor and looks forward to working with the students here.

A reception hosted by Miho and **Josh Sakon** was held August 12 for Margaret and Stefan at Sakon's house.

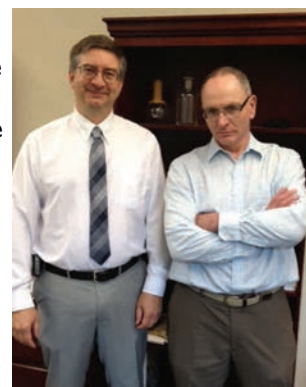




## Changes in the Department



**Dan Davis** and **Bill Durham**, former chair and vice-chair, were surprised with a departmental reception to thank them for their tenure leading the department. Dr. **Wesley Stites** assumed the chairmanship August 18, after serving as the department's vice-chair for 7 weeks. Wes Stites has been at the University of Arkansas since 1991. He grew up about a mile from the Arkansas River, but a few miles upstream from Fayetteville in Canon City, Colorado. Prior to returning to the vicinity of the Arkansas River, he was a post-doctoral fellow at Johns Hopkins University School of Medicine and received his Ph.D. from MIT in 1988. He wrote the successful NIH grant proposal which catalyzed the renovation of the Chemistry building and worked on that project



from 2000 to 2008. More recently, he just finished up a term of service on the Army Science Board. There are a number of challenges facing the department, for example, falling federal funding rates are worrying and accommodating the increase in the number of undergraduates both in infrastructure needs and recruiting new faculty will be time consuming and expensive. Nevertheless, Dr. Stites expressed confidence in the future. "The department has never been better and stronger in terms of buildings, instrumentation, and, most importantly, people. Whatever difficulties we have are no worse than what has been handled before. And we have some tremendous opportunities. I am looking forward to working with the rest of the faculty, staff and our great students to further improve the department and the university."

**Matt McIntosh** will serve as vice-chair alongside Wes. Dr. McIntosh is starting his 19th year at UA, having arrived in the department in 1996. He was tenured in 2002 and promoted to professor in 2011. He is also currently the Program Chair of the ACS Division of Organic Chemistry. For the 2014-15 academic year, Matt is a member of the college cabinet and the faculty senate, hence he encourages feedback from the CHBC faculty about issues at any level.

## Student News



**Kola Ayinuola** represented the department at the Networking Social with Graduate School Recruiters for undergrads at the ACS national meeting in San Francisco. The diverse research areas and extremely competitive funding available in the department were a big draw as well as the beautiful Ozark region.

Kola is a graduate student in Dr. Matt McIntosh's lab.



**Dr. Feng Wang** is pictured at left with post-docs **Hongyi Hu**, **Saieswari Amaran**, and **Jicun Li**, while climbing to 12,750 feet on the See Forever Trail at Telluride, Colorado. The group was attending the American Conference on Theoretical Chemistry, July 20-25. Please see the "On the Go" section on page 2 for a listing of their presentations.

## Alumni News

**Maha Shrestha**, Ph.D. 2013, has accepted an offer from Pittsburg State University, Pittsburg, KS as a Faculty/Research Associate (where she completed her MS degree). This is a unique opportunity to teach in the Department of Chemistry and work at Kansas Polymer Research Center (KPRC) at the same time. She is very happy to be back at PSU. Maha's U of A advisor was Dr. Matthias McIntosh.



**Stella Huff Nuckels**, Ph.D. 2009, and her husband **Craig Nuckels** announce the birth of their son **Michael Edward Nuckels**, born July 10, 2014. This picture was taken at his recent baptism. Stella is an Asst. Professor at Middle Georgia College. Her U of A advisor was Dr. Peter Pulay.

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## Safety Tip: by Bill Durham

A suggestion: Pick some aspect of lab safety and focus on that each month. For September, take a few minutes to check the Eye Wash Station. Clean and remove clutter from around the station. Make sure your inspection tag is up to date.



Department of Chemistry  
and Biochemistry

## Excellence in the Central Science

### Graduate Students Attend Conclave

**Marlena Patrick** and **Sarah Phillips** represented the University of Arkansas Alpha Sigma chapter at the 52nd Biennial Conclave for the national professional chemistry fraternity, Alpha Chi Sigma, in Charlottesville, VA. Pictured below are Sarah (l) and Marlena (r) with Colonel William Myers, esteemed retired faculty in the Department of Chemical Engineering at the U of A, as well as the alumni secretary for the Alpha Sigma chapter.



The department of chemistry and biochemistry at the University of Arkansas strives for excellence in research, teaching and service in chemistry - the central science. We aspire to positions of leadership regarding the discovery of new scientific knowledge, the training of students, and the economic development of the State of Arkansas. We seek to recruit and retain a diverse group of the best faculty, students and staff to address the challenges of the future through interdisciplinary and multidisciplinary research and education.

### Calendar of Events

#### September

- 01 Labor Day Holiday
- 08 Seminar, Dyhan Chandra, Roswell park Cancer Institute
- 12 CUME - 5:30-6:30, CHEM 144
- 15 Seminar, Qing Lin, University at Buffalo
- 26 CUME
- 29 Seminar, Steven Sucheck, University of Toledo

### Library Hours

CHBC Library (CHEM 225)  
<http://libinfo.uark.edu/chemistry>

#### Fall Semester Hours: August 24-December 19

##### Regular Fall Hours

Saturday and Sunday	CLOSED
Monday – Thursday	8:00 am – 9:00 pm
Friday	8:00 am – 6:00 pm

##### Exceptions to Regular Fall Hours

Monday	Sept 1 (Labor Day)	CLOSED
Friday	Oct 17	8:00 am - 5:00 pm
Mon-Tues	Oct 20-21 (Fall Break)	8:00 am - 5:00 pm
Tues-Wed	Nov 25-26	8:00 am - 5:00 pm
Thurs-Fri	Nov 27-28 (Thanksgiving)	CLOSED
Friday	Dec 19	8:00 am - 5:00 pm
<b>Interim &amp; Winter Break: December 20-January 2</b>		
Saturday – Sunday	Dec 20-21	CLOSED
Monday – Tuesday	Dec 22-23	8:00 am – 5:00 pm
Wednesday - Friday	Dec 24-Jan 2	CLOSED

The chemistry and biochemistry library resources can be accessed in the following LibGuides: <http://uark.libguides.com/content.php?pid=110953>. Please bookmark for future use.

### CUME Dates Announced

#### Fall CUME Dates:

September 12  
September 26  
October 10  
November 14  
December 5

5:30-6:30 p.m., CHEM 144

#### Spring CUME Dates:

January 23  
February 13  
March 13  
April 3  
April 24

TIME & PLACE TBA



#### Save the Date!

The 2014 INBRE conference will be held November 7-8 in Fayetteville, AR.

